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IDENTIFICATION OF NONLINEAR COEFFICIENT IN A TRANSPORT EQUATION

Abstract. Considered a problem of identification a nonlinear coefficient in a first order PDE via final observation. The problem is stated as an optimal control problem and solved numerically. Implicit finite difference scheme is used for the approximation of the state equation. A space of control variables is approximated by a sequence of finite-dimensional spaces with increaing dimensions. Finite dimensional problems are solved by a gradient method and numerical results are presented.

1. Introduction

In this paper we consider the following nonlinear initial boundary-value problem

$$\begin{cases} \dfrac{\partial c}{\partial t} + \dfrac{\partial c}{\partial x} + \dfrac{\partial a(c)}{\partial t} = 0, \quad x \in (0,1),\ 0 < t \leq T, \\ c(0,t) = 1, \\ c(x,0) = 0 \end{cases} \tag{1}$$

which models a convective transport of sorption chemical through a porous medium. Here c is the dissolved concentration of a chemical and $a(c)$ is a so-called sorption isotherm. Function $a(c)$ is the unknown of the problem, so we consider a structure identification problem. For

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physical reasons we assume $a(c)$ to be continuous and non-decreasing and $a(0) = 0$. Under these assumptions there exists a unique solution $c(x,t)$ to the problem (1) which takes its values from segment $[0,1]$. In order, to define $a(c)$ on $[0,1]$, we use a final observation $\phi(x)$: we try to choose $a(c)$ in such a way that $a(c(x,T)) = \phi(x)$, $(x \in [0,1])$, and where $\phi(x)$ is a non-negative continuous function. It is obvious that the formulated inverse problem is ill-posed, because it is not solvable for the arbitrary function $\phi(x)$.

We set up the above problem as an optimal control problem [5]. This approach is well-known in parameter identification problems (e.g. [1], [2]) and it is often called the output least squares method (cf. [3], [4]). In this paper we will concentrate on the numerical solution to the problem rather than its theoretical study.

In order to solve the optimal control problem we approximate the set of admissible coefficients $a(c)$ by a finite dimensional set. We also approximate problem (1) by a finite difference scheme. The existence of an unique solution to the finite-dimensional optimal control problem is shown. We use a gradient-type method for its solution, where the gradient information is calculated via the solution of an adjoint state problem. Due to the highly ill-posedness of the problem we chose an approach which is characterized by increasing the dimension of the set for admissible coefficient (cf.[4]). The results of the numerical experiments are presented.

2. Formulation of the problem and its discretization

We consider problem (1) with non-linear "coefficient" $a(c)$ which belongs to the following subset of the Lipshitz-continuous on $[0,1]$ functions:

$$A = \{a(c) \in C^{(0,1)}[0,1] : a(0) = 0, \frac{da}{dc} \geq 0 \text{ for a.a. } c \in [0,1]\}. \qquad (2)$$

Let us define the cost functional for the control optimization problem by

$$J(c) = \frac{1}{2}\int_0^1 (a(c(x,T)) - \phi(x))^2 dx. \qquad (3)$$

The problem under consideration can be posed as the following optimal control problem:

find $a(c) \in A$ such that it minimizes $J(c)$ when $c(x,t)$ satisfies the initial boundary-value problem (1).

Now in order to solve and stabilize the above stated optimal control problem we approximate the set A by a finite-dimensional set A_h. A_h is constructed by discretization of the coefficient space. Namely, let $a_h(c) \equiv a(u,c) = \sum_{i=1}^{N_u} u_i\psi_i(c)$, where the functions $\psi_i(c)$ compose a basis of a finite-dimensional space U_h, containing A_h, while $u = \{u_1, \dots, u_{N_u}\}^T$ belongs to a set $\mathcal{K}$ of admissible parameters: $u \in \mathcal{K} \Leftrightarrow a_h(c) \in A_h$. After an approximation of set A we derive the problem of minimization to the functional

$$I(u) \equiv J(u,c) = \frac{1}{2}\int_0^1 (a(u,c(x,T)) - \phi(x))^2 dx \tag{4}$$

with $c = c(u)$ satisfying (1) and $u \in \mathcal{K}$.

For the differentiable function $a(u,c) \in A_h$ the functional $I(u)$ is also differentiable and

$$\nabla I(u) = \int_0^1 (a(u,c(x,T)) - \phi(x))a'_u(u,c(x,T))dx + \int_0^T\int_0^1 \frac{\partial}{\partial t}a'_u(u,c(x,t))\lambda(x,t)dxdt. \tag{5}$$

Here $c(x,t)$ is the solution of the state problem (1) and $\lambda(x,t)$ is the solution of the corresponding adjoint problem:

$$\begin{cases} \displaystyle\int_0^T ((1 + a'_c(u,c(x,t))\frac{\partial\lambda}{\partial t} + \frac{\partial\lambda}{\partial x})\mu(x,t)dxdt \\ \displaystyle\qquad = \int_0^1 (1 + a'_c(x,T)\lambda(x,T)\,\mu(x,T))dx \\ \displaystyle\qquad\qquad + \int_0^T \lambda(1,t)\,\mu(1,t)dt \\ \displaystyle + \int_0^1 (a(u,c(x,T)) - \phi(x))a'_c(u,c(x,T)\mu(x,T)dx, \\ \qquad\qquad \forall\mu(x,t) : \mu(0,T) \equiv \mu(x,0) \equiv 0. \end{cases} \tag{6}$$

We can rewrite (6) in pointwise form:

$$\begin{cases} (1+a_c'(u,c))\dfrac{\partial\lambda}{\partial t}+\dfrac{\partial\lambda}{\partial x}=0, \quad 0<x<1, \;\; 0<t\le T,\\ \lambda=0, \qquad x=1, 0<t\le T\\ (1+a_c'(u,c))\lambda+(a(u,c)-\phi(x))a_c'(u,c)=0, \quad 0<x<1, \;\; t=T. \end{cases}$$

In order to solve numerically the optimal control problem we discretize the state problem (1) and construct corresponding discrete adjoint state problem. Let us divide the segment $[0,1]$ by the uniform mesh with stepsize $h_u=1/N_u$, $N_u\in\mathcal{N}$, and define finite-dimensional spaces

$$U_h=\{a(c) : a(c) \text{ is piecewise linear and continuous on } [0,1], a(0)=0\}$$

and

$$A_h=\{a(c)\in U_h: \; a(ih_u)\le a((i+1)h_u) \text{ for all } i=0,1,...,N_u\}.$$

Now we consider set $\{\psi_i(c)\}_{i=1}^{N_u}$ which is the basis of U_h. This set consists of the piecewise polynomial functions which are defined the following way:

$$\psi_i(c)=\begin{cases} 0 & for \quad 0\le c\le (i-1)h_u\\ N_u(c-(i-1)h_u) & for \quad (i-1)h_u<c\le ih_u\\ 1 & for \quad ih_u<c\le 1 \end{cases} \tag{7}$$

Use of the basis (7) instead of usual Courant basis allows us to obtain the simplest form of the set A_h via the nodal parameters of the functions $a(c)\in A_h$:

$$a(c)\equiv a(u,c)=\sum_{i=1}^{N_u}u_i\psi_i(c) \text{ iff } u\in\mathcal{K}\equiv(\mathcal{R}^{N_u})^+.$$

Now, let $\bar\omega=\{x_i=ih, i=0,1,..,N\}$ be an uniform mesh on $[0,1]$ with mesh step-size h and $\omega^+=\bar\omega\setminus\{x_0\}$. We also introduce $\bar\omega_\tau=\{t_k=k\tau, k=0,1,..,N_\tau\}$ being uniform mesh on $[0,T]$ with step-size τ, $\omega_\tau^+=\bar\omega_\tau\setminus\{t_0\}$, $\omega_\tau^-=\bar\omega_\tau\setminus\{t=T\}$.

We define the finite differences in time as:

$$v_{\bar t}=\frac{1}{\tau}(v(x,t)-v(x,t-\tau)), \;\; v_t=\frac{1}{\tau}(v(x,t+\tau)-v(x,t))$$

and in space as:

$$v_{\bar x}=\frac{1}{h}(v(x,t)-v(x-h,t)), \;\; v_x=\frac{1}{h}(v(x+h,t)-v(x,t)).$$

State equation (1) is approximated by the following implicit scheme:

$$\begin{cases} (c_h + a_h)_{\bar{t}}(x,t) + c_{h\bar{x}}(x,t) = 0 \text{ for } x \in \omega^+,\ t \in \omega_\tau^+, \\ c_h(0,t) = 1, \quad \text{for } t \in \bar{\omega}_\tau, \\ c_h(x,0) = 0 \quad \text{for } x \in \omega^+, \end{cases} \tag{8}$$

where $a_h = a(u, c_h)$. Applying the quadrature formula to (4), we derive the following finite-dimensional cost functional:

$$I(u) \equiv J_h(u, c_h) = \sum_{i=1}^{N} (a(u, c_i) - \phi(x_i))^2, \tag{9}$$

where $c_i = c_h(x_i, T)$.

Futher we consider the optimal control problem (OCP):

$$\textit{find } \min J_h(u, c_h) \textit{ for } u \in \mathcal{K}, \textit{ when equation (8) is fulfilled.} \tag{10}$$

Lemma 1. *Discretization scheme (8) has a unique solution $c_h(x,t)$ for any $u \in \mathcal{K}$, and $0 \le c_h(x,t) \le 1$ for all $x,\ t$.*

Proof. For a fixed time level t problem (8) can be written as

$$(1+\frac{\tau}{h})c_h(x,t)+a(u,c_h(x,t)) = c_h(x,t-\tau)+a(u,c_h(x,t-\tau))+\frac{\tau}{h}c_h(x-h,t).$$

Because $c_h(0,t) = 1$, we solve recurrently the equations with monotone increasing and continuous functions to find $c_h(x,t)$ for all $x \ge h$, whence the unique solvability follows. Further, owing to the non-negativeness of the initial and boundary conditions we obviously have $c_h(x,t) \ge 0$. Now, let $c_h(x, t-\tau) \le 1$ and $c_h(x,t) \le 1$ for $x \le x_i$. If we suppose that $c_h(x_{i+1}, t) > 1$, then from (8) it follows $(c_h + a_h)_{\bar{t}}(x_{i+1}, t) < 0$, thus, $c_h(x_{i+1}, t) < c_h(x_i, t)$ and we get a contradiction. $\square$

In addition, we prove that c_h is a Lipschitz-continuous function of u. To do this we rewrite equation (8) for a fixed time level in an algebraic form. Let $c = c(t) = c(t,u) \in \mathcal{R}^N$ be the vector of nodal values to $c_h(x,t) : c_i = c_h(x_i,t)$ for $i = 1,\dots,N$, while $f = f(u) \in \mathcal{R}^N$ be the vector with coordinates $f_i = c_h(x_i, t-\tau) + a(u, c_h(x_i, t-\tau))$ for $i = 2,\dots,N$ and $f_1 = c_h(x_1, t-\tau) + a(u, c_h(x_1, t-\tau)) + \tau/h$. Let further $B \in \mathcal{R}^{N\times N}$ be the two-diagonal matrix with diagonal elements $1 + \tau/h$ and off-diagonal ones $-\tau/h$. Then (8) for a fixed time level t has the form

$$Bc + a(u,c) = f(u). \tag{11}$$

Lemma 2. *Let $c(u) \equiv c(t,u)$ and $c(v) \equiv c(t,v)$ be the solutions of (11), corresponding to $u,\ v \in \mathcal{K}$. Then there exists a constant $M = M(t,u)$ such that*

$$||c(t,u) - c(t,v)||_\infty \leq M||u-v||_1, \tag{12}$$

where $||.||_\infty$ and $||.||_1$ are maximum and L_1-norm of vectors, respectively.

Proof. Let I be unit matrix and $\sigma = \sigma(u) = \sum_{j=1}^{N_u} u_j N_u$. From equation (11) we obtain

$$c(u) = (B + \sigma I)^{-1}(\sigma c(u) - a(u, c(u)) + f(u)),$$
$$c(v) = (B + \sigma I)^{-1}(\sigma c(v) - a(v, c(v)) + f(v))$$

and estimate the difference

$$\begin{aligned} c(u) - c(v) & \\ &= (B+\sigma I)^{-1}(\sigma(c(u)-c(v)) - a(u,c(u)) + a(u,c(v)) \\ &\quad + (B+\sigma I)^{-1}(f(u) - f(v) + (a(v,c(v)) - a(u,c(v))) \\ &= (B+\sigma I)^{-1}(\sum_{j=1}^{N_u} u_j(N_u(c(u)-c(v)) + \psi_j(c(v)) - \psi_j(c(u))) \\ &\quad + (B+\sigma I)^{-1}(f(u) - f(v) + \sum_{j=1}^{N_u}(v_j - u_j)\psi_j(c(v))). \end{aligned} \tag{13}$$

Let L_j be the diagonal matrix with entries, defined the following way: if $c_i(u) \neq c_i(v)$ then the i-th diagonal entry of L_j is $\dfrac{\psi_j(c_i(u)) - \psi_j(c_i(v))}{c_i(u) - c_i(v)}$; otherwise it is equal to 0. With this definition one has

$$\psi_j(c(u)) - \psi_j(c(v)) = L_j(c(u) - c(v)). \tag{14}$$

Owing to the definition of the functions ψ_j

$$0 \ll L_j \ll N_u I, \tag{15}$$

where by $\ll$ the componentwise inequality is denoted. From (14) and (15) we obtain

$$\begin{aligned} &|\sum_{j=1}^{N_u} u_j(N_u(c(u)-c(v)) + \psi_j(c(v)) - \psi_j(c(u))| \ll \\ &\sum_{j=1}^{N_u} u_j|(L_j - N_u I)(c(u)-c(v))| \ll \sigma|(c(u)-c(v))|. \end{aligned} \tag{16}$$

Direct calculations show that

$$||(B+\sigma I)^{-1}||_\infty \le \frac{1}{1+\sigma}. \tag{17}$$

Now, (13), (16) and (17) yield

$$||c(u)-c(v)||_\infty \le (1+\sigma)||(B+\sigma I)^{-1}(f(u)-f(v)+\sum_{j=1}^{N_u}(v_j-u_j)\psi_j(c(v)))||_\infty$$

$$\le ||f(u)-f(v)||_\infty + \sum_{j=1}^{N_u}|v_j-u_j|.$$

Because $f(u)-f(v) = c(t-\tau,u)-c(t-\tau,v)+a(u,c(t-\tau,u))-a(v,c(t-\tau,v))$ and similarly to the previous estimates we have

$$|a(u,c(t-\tau,u))-a(v,c(t-\tau,v))| \ll \sigma|c(t-\tau,u)-c(t-\tau,v)|+||u-v||_1,$$

then

$$||f(u)-f(v)||_\infty \le (1+\sigma)||c(t-\tau,u)-c(t-\tau,v)||_\infty + ||u-v||_1.$$

Thus,

$$||c(t,u)-c(t,v)||_\infty \le (1+\sigma)||c(t-\tau,u)-c(t-\tau,v)||_\infty + 2||u-v||_1,$$

whence inequality (12) follows with $M(t,u) = 2\dfrac{(1+\sigma(u))^{t/\tau}}{\sigma(u)}$. □

Theorem 1. *Problem (10) has a solution for any* $u \in \mathcal{K}$

Proof. Owing to the previous Lemma 2 and definition of $a(u,c)$, the cost function $I(u)$ is continuous, and obviously it is coercive: $||u|| \to \infty \Rightarrow I(u) \to +\infty$, whence the result. □

3. Iterative method

A function $a(u,c_h) \in A_h$ is not differentiable in c_h. However, it is Lipcshitz-continuous and has left and right derivatives a'_c. Below we use the piecewise constant function a'_c (by taking either left or right derivative) to construct adojnt state and to receive "gradient" information. To construct the adjoint state problem we define the following Lagrange function

$$L_h(u,c_h,\lambda_h) = J_h(u,c_h)+\tau\sum_{t\in\omega_\tau^+} h \sum_{x\in\omega^+} \lambda_h(x,t)((c_h+a_h)_{\bar t}(x,t)+c_{h\bar x}(x,t)), \tag{18}$$

where the mesh function $\lambda_h(x,t)$ vanishes when $x=0$ or $t=0$. Stationary points of Lagrange function L_h are defined from the following system

$$\nabla_\lambda L_h \cdot \delta\lambda_h \equiv \tau \sum_{t\in\omega_\tau^+} h \sum_{x\in\omega^+} ((c_h+a_h)_{\bar t}(x,t) + c_{h\bar x}(x,t))\delta\lambda_h(x,t) = 0; \quad (19)$$

$$\nabla_c L_h \cdot \delta c_h \equiv h \sum_{x\in\omega^+} (a(u, c_h(x,T)) - \phi_h(x)) a'_c(u, c_h(x,T))\delta c_h(x,T)$$

$$+\tau \sum_{t\in\omega_\tau^+} h \sum_{x\in\omega^+} ((\delta c_h + a'_c \delta c_h)_{\bar t}(x,t) + (\delta c_h)_{\bar x}(x,t))\lambda_h(x,t) = 0; \quad (20)$$

$$\nabla_u L_h \cdot \delta u \equiv h \sum_{x\in\omega^+} (a(u, c_h(x,T)) - \phi_h(x)) a'_u(u, c_h(x,T))\delta u$$

$$+\tau \sum_{t\in\omega_\tau^+} h \sum_{x\in\omega^+} \lambda_h(x,t)(a'_u)_{\bar t}(x,t)\delta u = 0, \quad (21)$$

where $\delta u \in \mathcal{R}^m$ and trial mesh functions $\delta\lambda_h$ and δc_h vanish when $x=0$ or $t=0$.

Equation (20) gives us the adjoint state problem which has the following pointwise form

$$\begin{cases} -(1+a'_c)\lambda_t - \lambda_x = 0, & 0<x<1, \quad t\in\omega_\tau^-, \\ -(1+a'_c)\lambda_t + \frac{1}{h}\lambda_x = 0, & x=1, \quad t\in\omega_\tau^-, \\ (1+a'_c)\lambda - \tau\lambda_x + a'_c(a-\phi) = 0, & 0<x<1, \quad t=T, \\ (1+a'_c)\lambda + \frac{\tau}{h}\lambda_x + a'_c(a-\phi) = 0, & x=1, \quad t=T. \end{cases} \quad (22)$$

From the equation (21) we derive the formula for calculation the gradient $\nabla I(u) = \nabla_u L_h$:

$$\nabla I(u) = h \sum_{x\in\omega^+} (a(u, c_h(x,T)) - \phi_h(x)) a'_u(u, c_h(x,T))$$

$$+\tau \sum_{t\in\omega_\tau^+} h \sum_{x\in\omega^+} \lambda_h(x,t)(a'_u)_{\bar t}(x,t) \quad (23)$$

Now to minimize the functional $I(u)$ we use the gradient method:

$$u^{k+1} = u^k - \rho_{k+1}\nabla I(u^k), \quad (24)$$

where an initial guess $u^0 \in \mathcal{K}$, and iterative parameter ρ_{k+1} is defined via the line search technique. To improve the convergence of the method we use “multilevel” implementation; namely, we first solve the problem with the dimension $N_u = 2$ of the space U_h and then increase N_u. This approach gives us the possibility to achieve better results than if using fixed dimension N_u.

4. Numerical results

In this section, we will describe numerical experiments that we have performed for the solution of the above defined optimal control problem.

We discretize domain $\Omega = (0, L) \times T$ by uniform mesh with step size h and time step Δt. Then, we define discrete control space U_h with the dimension N_u. For the numerical experiments we have used the following objective functions ϕ:

$$\phi_1(x) = 0.5(1.0 - x),$$

$$\phi_2(x) = \begin{cases} 1, & 0 \leq x \leq L/2, \\ 0, & L/2 < x \leq L, \end{cases}$$

$$\phi_3(x) = \begin{cases} 0.5 - x, & 0 \leq x \leq L/2, \\ 0, & L/2 < x \leq L. \end{cases}$$

We have performed calculations for variable $N_u = 2, 4, 8, 16, 32$, where on each step after increasing N_u we used the previous solution as an initial data.

Figures 1 - 6 show evaluated coefficient $a(c)$ and comparison between objective function ϕ and computed values of $a(c(x, T))$ for three considered functions ϕ and for different mesh and time step sizes.

Remark 1. *We also performed calculations "directly" for $N_u = 32$ without multilevel approach. The calculated results were similar to the previous ones, but the number of iterations and especially the time of calculation were much greater than for the multilevel method.*

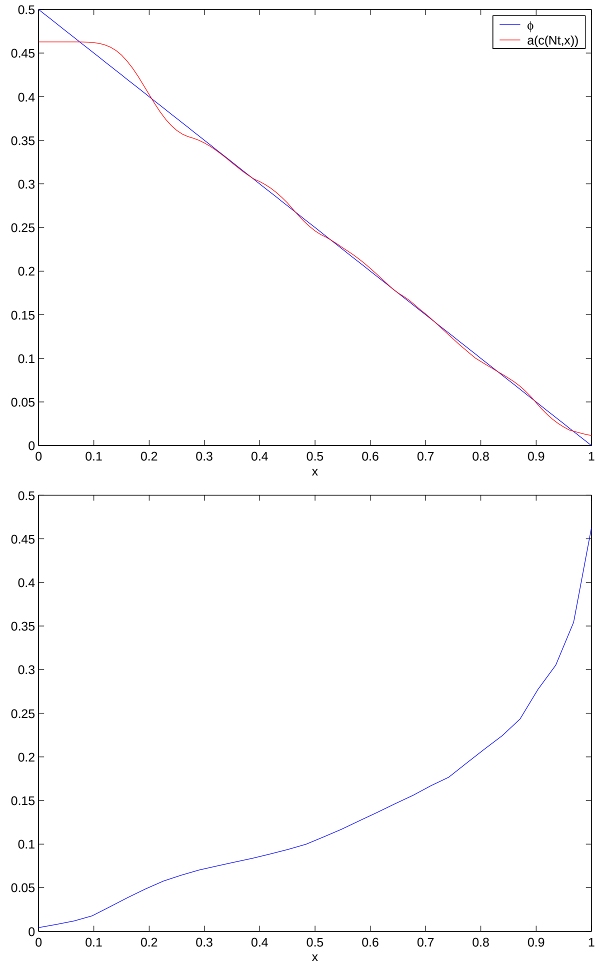

FIGURE 1. Objective function ϕ_1 and calculated $a(c(x,T))$ (top) and computed nonlinear coefficient $a(c)$ (bottom) for $h = \tau = 0.01$

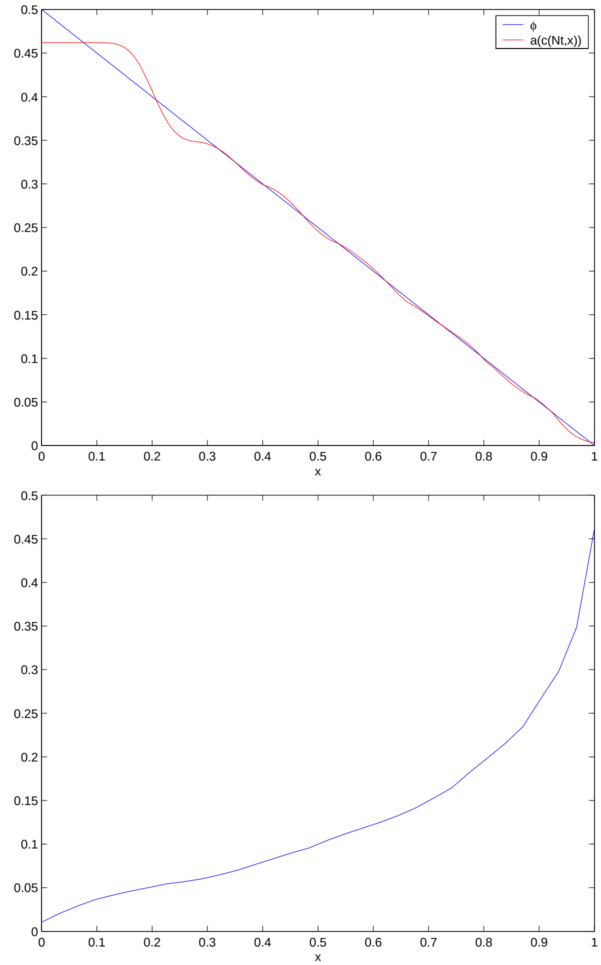

FIGURE 2. Objective function ϕ_1 and calculated $a(c(x,T))$ (top) and computed nonlinear coefficient $a(c)$ (bottom) for $h = \tau = 0.005$

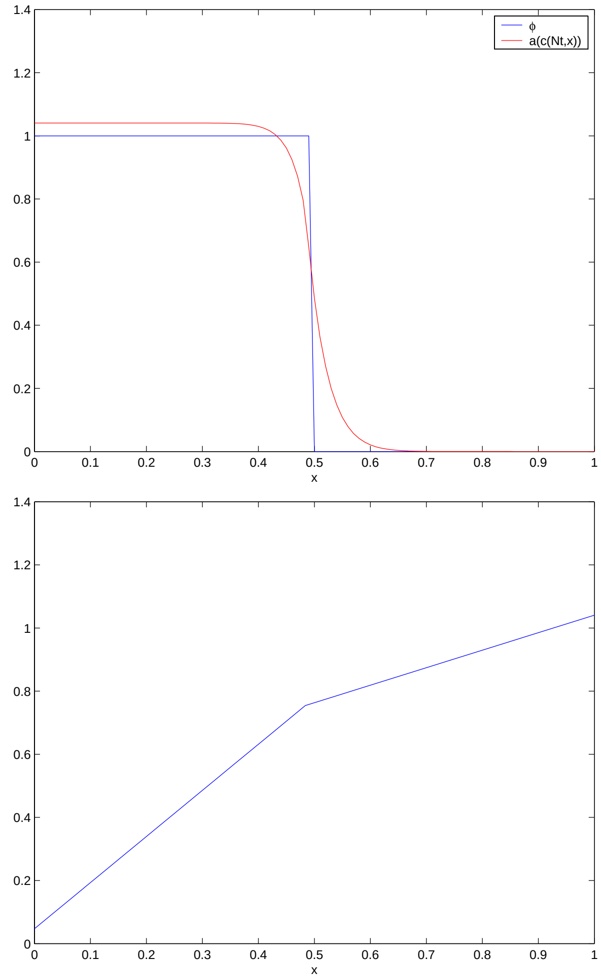

FIGURE 3. Objective function ϕ_2 and calculated $a(c(x,T))$ (top) and computed nonlinear coefficient $a(c)$ (bottom) for $h = \tau = 0.01$

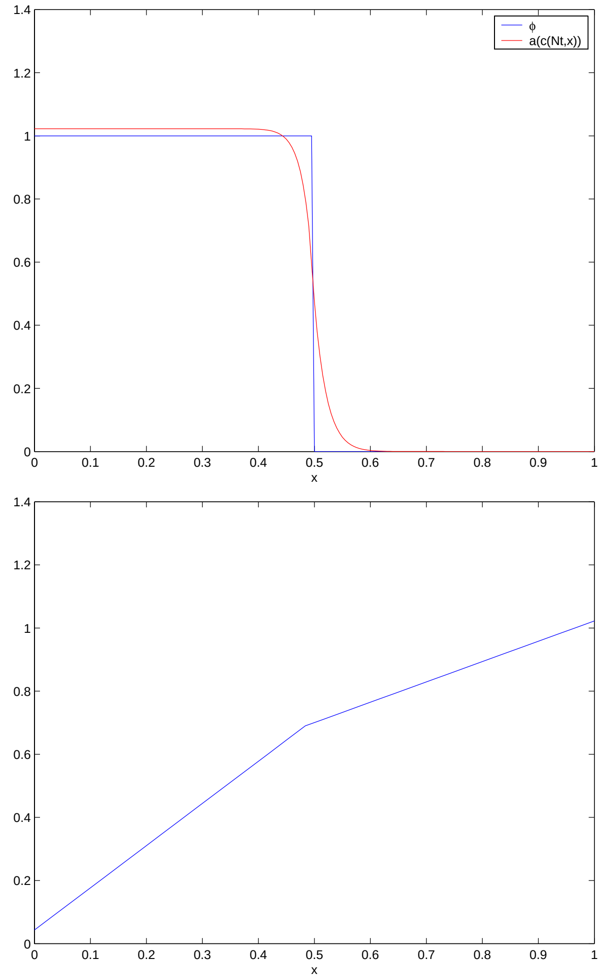

FIGURE 4. Objective function ϕ_2 and calculated $a(c(x,T))$ (top) and computed nonlinear coefficient $a(c)$ (bottom) for $h = \tau = 0.005$

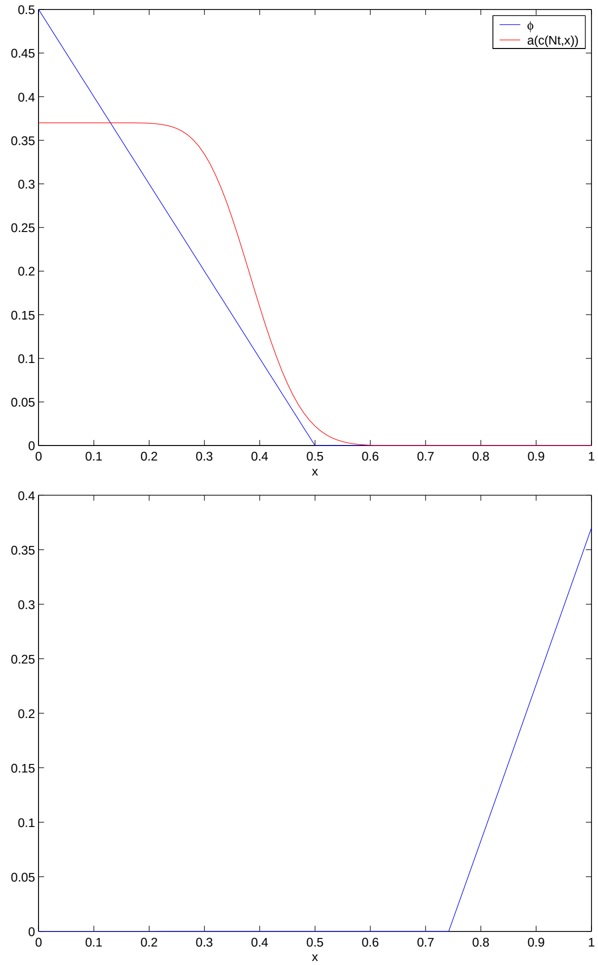

FIGURE 5. Objective function ϕ_3 and calculated $a(c(x,T))$ (top) and computed nonlinear coefficient $a(c)$ (bottom) for $h = \tau = 0.01$

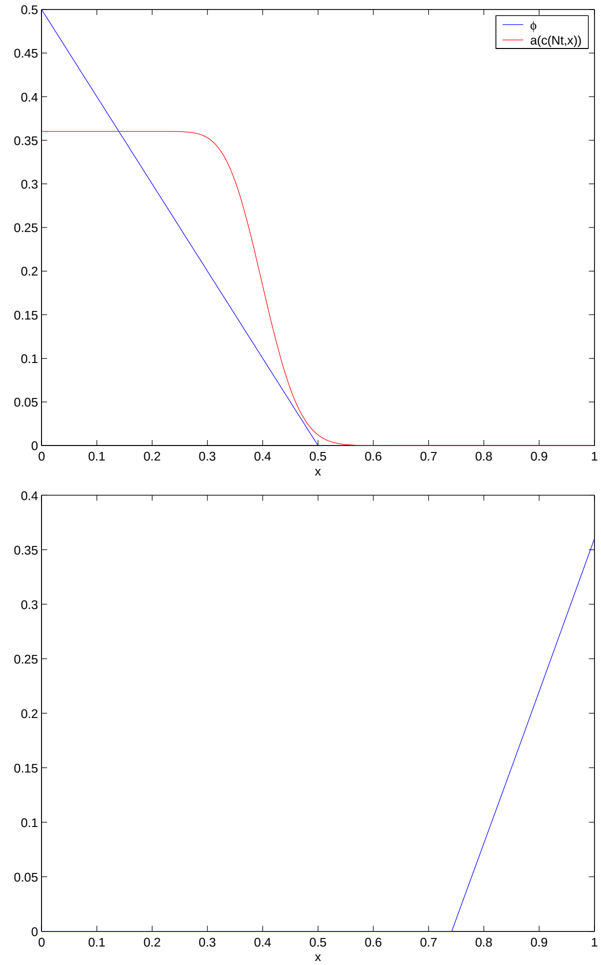

FIGURE 6. Objective function ϕ_3 and calculated $a(c(x,T))$ (top) and computed nonlinear coefficient $a(c)$ (bottom) for $h = \tau = 0.005$

References

[1] Chavent G., Lemonnier P., *Identification de la Non-Linearité D'Une Équation Parabolique Quasilineaire* Applied Mathematics and Optimization, Springer Verlag, 1974, vol.1, No.2,pp.121-162

[2] DuChateau P. *An Inverse Problem for the Hydraulic Properties of Porous Media*, SIAM J. Math. Analysis, 1997, Vol.28, No.3, pp.611-632

[3] Igler B., Totsche K.U., Knabner P. *Unbiased Identification of Nonlinear Sorption Characteristics by Soil Column Breakthrough Experiments*, Preprint IAM Erlangen, 1997, No. 224

[4] Knabner P., Igler B. *Structural Identification of Nonlinear Coefficient Functions in Transport Processes through porous media*, in Lectures on Applied Mathematics, Springer Verlag, 2000, pp.157-178

[5] Lions J.L.*Optimal Control of Systems Governed by Partial Differential Equations*, Springer Verlag, New York, 1971

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